Antiferromagnetic and spin gap phases of the anisotropic Kondo necklace model

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We have studied the effect of anisotropies on the quantum phase transition of the Kondo necklace model in dimensions D=1, 2 and 3. Both the anisotropy δ of the inter-site interaction term and anisotropy Δ of the on-site Kondo interaction have been included. We use a bond operator method with constraints implemented in mean field approximation. Starting from the paramagnetic phase we determine the critical ratio $(t/J)_c$ of the quantum critical point and associated scaling exponents of the Kondo-singlet gap. We show that in the case of easy-axis type anisotropy $\delta > 1$ a qualitatively new behavior in comparison to the conventional Kondo necklace model with $(\delta,\Delta)=(0,1)$ appears. We have also obtained the antiferromagnetic order parameter in the long range ordered phase for $t > t_c$.

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I. INTRODUCTION

Quantum phase transitions in heavy fermion systems between a Fermi liquid and antiferromagnetically (AF) ordered state have been at the focus of research recently [1, 2]. This is due to mainly two reasons: Firstly in the vicinity of the quantum critical point (QCP) which is usually reached by applying external or doping-induced chemical pressure, the intrinsic energy scale of the compound, i.e., effective Fermi temperature T^* or Néel temperature T_N vanishes. This leads to a breakdown of the Fermi liquid picture and non-Fermi liquid behavior of thermodynamic and transport quantities is observed close to the QCP [3]. It is therefore of great interest to understand the approach to the quantum critical region within suitable theoretical models. The most important among them is the Kondo lattice model consisting of a free conduction band and an on-site AF Kondo interaction which favors nonmagnetic singlet formation. In the second order it also leads to the effective inter-site RKKY interactions which favor magnetic order. Their competition leads to the appearance of the QCP. In such a picture only spin degrees of freedom are involved in the quantum phase transition. Therefore the Kondo lattice model may be replaced by a simpler model where the itinerant hopping part is simulated by an inter-site interaction of the itinerant spins. In the work of Doniach [4] it was shown that in dimension D=1 this replacement, leading to the 'Kondo-necklace' model is indeed exact assuming that the inter-site interaction is of the XY-type. Later more general anisotropic inter-site interactions have been considered including the z-component of conduction-electron spins [5]. In the itinerant picture this would be equivalent to adding an interaction term for conduction electrons, i.e., considering Kondo spins that are screened by correlated conduction electrons [6]. In addition the Kondo-necklace model was considered in higher dimension [7]. In this case the direct connection to the original itinerant Kondo lattice model is lost. One then has to consider the Kondo necklace model for D ≥ 2 as a model in its own right. In fact exact diagonalisation results [9] for finite clusters show that the two models are still closely related even for D = 2.

In the present work we want to study the possible quantum phase transition in the D = 1-3 Kondo-necklace type model under rather general assumption of the anisotropy of both the inter-site interaction and on-site Kondo terms. They are characterised by the pair of parameters (δ, Δ). For the former $\delta \neq 0$ describes the deviation from the XY-type interaction associated with free conduction electrons in 1D and for the latter $\Delta \neq 1$ describes deviation from the isotropic on-site Kondo interaction. The Δ anisotropy is always present in real Kondo compounds like Ce-based intermetallics due to the crystalline electric field (CEF).

For uniaxial symmetry it splits the $J = \frac{5}{2}$ multiplet into a sequence of Kramers doublets. The ground state doublet $|\pm\rangle$ may be described by a pseudo-spin $S=\frac{1}{2}$. Projecting the Kondo term to this subspace then leads to different on-site exchange for $S_{x,y}$ and S_z components. This defines a local anisotropy ratio $\Delta = J_z/J_x$ of the pseudo-spin Kondo term. In real Kondo compounds this ratio may assume any value between the easy axis (Ising-like) case $\Delta \to \infty$ and the easy-plane (xy-like) case $\Delta = 0$. Examples of tetragonal compounds are $CeRu_2Si_2$ [10] for the former and $YbRh_2Si_2$ [11] for the latter.

We study the quantum phase transition from the paramagnetic (Kondo-singlet) side as function of the control paramter t/J giving the ratio of inter-site to on-site interaction strength and as function of the ansisotropies (δ,Δ). Previously this has only been performed in the special case $(\delta,\Delta)=(0,1)$ [7]. For the case of general (δ,Δ) we use the same bond operator representations of spin variables where on-site constraints are implemented in mean field approximation.
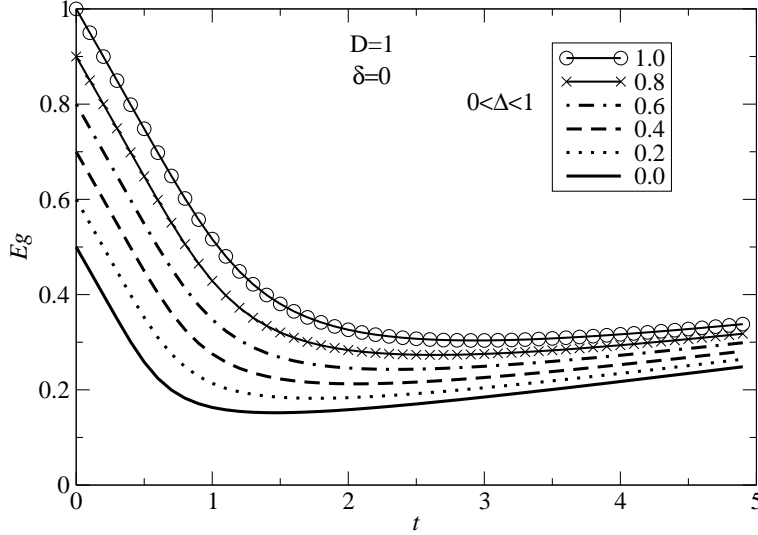
FIG. 1: The energy gap E_g versus hopping strength in the one dimensional lattice. Different plots show the effect of local anisotropy, $0 \leq \Delta \leq 1$.

In Sec. II we give a brief definition of the anisotropic Kondo necklace model and the bond-operator transformation. In Sec. III the ground state energy and excitation spectrum is calculated in mean field approximation. Using the numerical results the quantum phase transitions and phase diagrams are discussed in Sec. IV. The extension of the mean field approach for the antiferromagnetic ordered phase is presented in Sec. V. Finally Sec. VI gives the summary.

II. ANISOTROPIC KONDO NECKLACE MODEL

We investigate the anisotropic Kondo necklace model which is defined by the following Hamiltonian

$$H = H_t + H_J = t \sum_{<i,j>} (\tau_i^x \tau_j^x + \tau_i^y \tau_j^y + \delta \tau_i^z \tau_j^z) + J \sum_i (\tau_i^x S_i^x + \tau_i^y S_i^y + \Delta \tau_i^z S_i^z). \tag{1}$$

In the above Hamiltonian, τ_n^α represent the α-component of spin of the itinerant electron at site n and S_n^α is the α-component of localized spins at position n. For the exchange coupling between the itinerant and localized spins we have used $J_x \equiv J = 1$ as the reference energy scale in all figures. The hopping parameter of the itinerant electrons is proportional to t with the anisotropy in the z-direction given by δ. Therefore the above model has three control parameters: t/J and the anisotropies (δ, Δ). There are two main reasons for considering the anisotropy both in the itinerant and localized parts of the interactions: (i) In real materials where the Kondo effect has been observed there exists the anisotropy in the interaction between the localized and itinerant electrons. (ii) The anisotropy in the itinerant part of the interaction enables us to investigate the effect of symmetry on the results of the Kondo necklace model compared with the Kondo model. In the present model the case of $\delta \neq 1$ has $U(1)$ symmetry and for $\delta = 1$ it has $SU(2)$ symmetry, the same as in the genuine Kondo model. Moreover, in one dimensional lattice nonzero δ represents the interaction between itinerant electrons [12].

Our approach is based on the strong coupling limit $J/t \rightarrow \infty (t = 0)$ where the model is composed of independent pairs of spins $(\tau, \mathbf{S})$. The Hilbert space of a pair of spins consists of 4 states where it can be represented by a singlet and a triplet. This basis can be created out of the vacuum by singlet and triplet creation operators: $|s\rangle = s^\dagger |0\rangle$ and $|t\rangle = t_\alpha^\dagger |0\rangle$ $(\alpha = x, y, z)$. In terms of singlet-triplet operators the spin operator of the localized and conduction
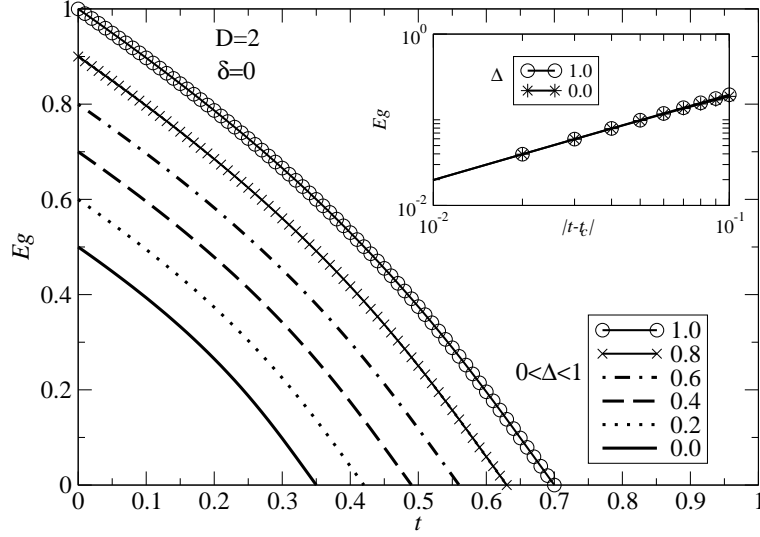
FIG. 2: The energy gap E_g versus hopping strength in the two-dimensional lattice for $\delta = 0$. The inset shows the log-log plot of E_g versus $|t - t_c|$ for $\Delta = 0, 1$ where the gap scales like $E_g \sim |t - t_c|^\nu$ with $\nu \simeq 1$ close to the critical point.

electrons are given by

$$S_{n,\alpha} = \frac{1}{2}(s_n^\dagger t_{n,\alpha} + t_{n,\alpha}^\dagger s_n - i\epsilon_{\alpha\beta\gamma} t_{n,\beta}^\dagger t_{n,\gamma}),$$

$$\tau_{n,\alpha} = \frac{1}{2}(-s_n^\dagger t_{n,\alpha} - t_{n,\alpha}^\dagger s_n - i\epsilon_{\alpha\beta\gamma} t_{n,\beta}^\dagger t_{n,\gamma}), \tag{2}$$

where (α, β, γ) represent the (x, y, z) components and ϵ is the totally antisymmetric tensor. This type of representation has been introduced first by Sachdev and Bhatt [13] called *bond operators*. The bond operators satisfy bosonic commutation relations $[s_n, s_n^\dagger] = 1$, $[t_{n,\alpha}, t_{n,\beta}^\dagger] = \delta_{\alpha,\beta}$ and $[s_n, t_{n,\beta}^\dagger] = 0$. The physical states are obtained by the local constraint $s_n^\dagger s_n + \sum_\alpha t_{n,\alpha}^\dagger t_{n,\alpha} = 1$. Using Eq.(2) the Hamiltonian (Eq.(1)) may be expressed in terms of bond operators. As discussed in the next section it then reduces to a simple form within the mean-field approximation.

III. SINGLET CONDENSATION AND GROUND STATE PROPERTIES IN MEAN-FIELD APPROXIMATION

We have followed the mean-field approach introduced in Ref.7 where the local constraint is replaced by a global one for the average amplitudes $\langle s_n \rangle$ and $\langle t_{n,\alpha} \rangle$. In this respect we start from the strong coupling limit $J/t \to \infty$ $(t = 0)$ where the ground state is composed of the direct product of local singlets. In this limit we have $\langle s_n \rangle = \langle s_n^\dagger \rangle = 1$ and $\langle t_{n,\alpha} \rangle = \langle t_{n,\alpha}^\dagger \rangle = 0$ where the ground state represents the pure condensation of local singlets. Turning on the hopping of conduction electrons $(t \neq 0)$ the triplet occupation at each site becomes nonzero but still very small as will be shown later. Thus, for a small value of t/J we consider a mean field value for $\langle s_n \rangle = \langle s_n^\dagger \rangle = \bar{s}$ and the excitations above this background are defined by the triplet states which define the mean field Hamiltonian. The hopping term of the Hamiltonian which is modeled by the XXZ interaction between the spin of conduction electrons will be written as a sum of three terms, i.e., $H_t = H_1 + H_2 + H_3$ associated with the different types of singlet and triplet interactions.
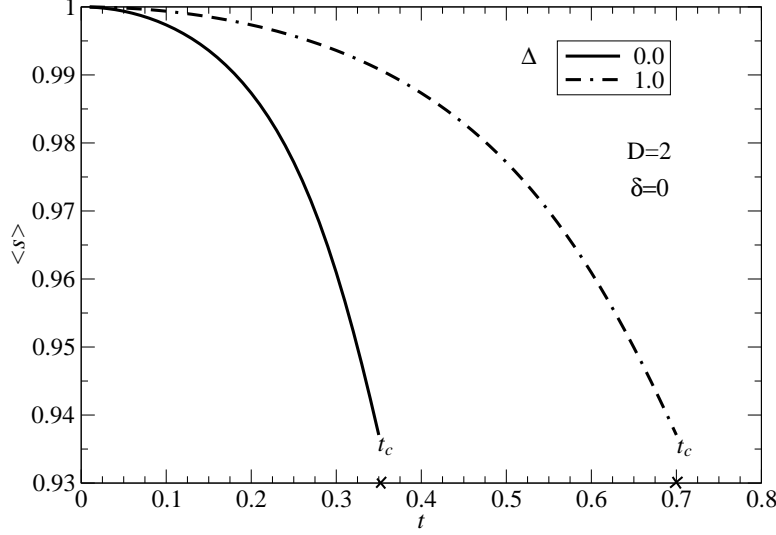
FIG. 3: The occupation of singlets in the ground state ($< s >= \bar{s}$) versus the hopping strength up to the critical point t_c for two different values of anisotropy $\Delta = 0, 1$ in the two dimensional lattice. The crosses ($\times$) indicate the critical point for each case. The deviation from fully occupied state ($< s >= 1$) is very small for $t < t_c$.

The first term is given by

$$H_1 = \frac{t}{4} \sum_{<n,m>} \sum_{\alpha=x,y} \left(s_n^\dagger t_{n,\alpha} (s_m^\dagger t_{m,\alpha} + t_{m,\alpha}^\dagger s_m) + h.c. \right) \tag{3}$$

$$+ \frac{t\delta}{4} \sum_{<n,m>} \left(s_n^\dagger t_{n,z} (s_m^\dagger t_{m,z} + t_{m,z}^\dagger s_m) + h.c. \right). \tag{4}$$

The explicit form of H_2 and H_3 are given in the appendix. However, H_2 contains the interaction between the triplet bosons which will have negligible effect on the result of considering only H_1 because the average triplet occupation is small. The contribution of H_3 to the ground state energy is identically zero in mean field approximation, since each term of H_3 consists of three triplets and one singlet operator.

The exchange term (H_J) is diagonal in terms of the bond operators,

$$H_J = \frac{J}{4} \sum_n \left(-(2+\Delta)s_n^\dagger s_n + (2-\Delta)t_{n,z}^\dagger t_{n,z} + \Delta(t_{n,x}^\dagger t_{n,x} + t_{n,y}^\dagger t_{n,y}) \right). \tag{5}$$

The physical constraint is imposed by adding a Lagrange term at each site with an associated chemical potential μ_n to the Hamiltonian

$$H = H_1 + H_J + \sum_n \mu_n (s_n^\dagger s_n + \sum_{\alpha=x,y,z} t_{n,\alpha} t_{n,\alpha}^\dagger - 1). \tag{6}$$

The mean field Hamiltonian, $H_{mf} = \langle H \rangle$ is obtained by taking $\langle s_n \rangle = \langle s_n^\dagger \rangle = \bar{s}$ and a global value for the chemical potential, $\mu_n = \mu$. After performing the Fourier transform and the Bogoliubov transformation the mean field Hamiltonian is written in the following form,

$$H_{mf} = E_0 + \sum_k \sum_{\alpha=x,y,z} \omega_\alpha(k) a_{k,\alpha}^\dagger a_{k,\alpha}. \tag{7}$$

In this equation, E_0 is the ground state energy, $\omega_\alpha(k)$ is the excitation energy of the new bosons defined by the number operator $a_{k,\alpha}^\dagger a_{k,\alpha}$. The new bosons can be expressed in terms of the bond operators via the Bogoliubov

transformations,

$$a_{k,\alpha} = \cosh(\theta_{k,\alpha})t_{k,\alpha} + \sinh(\theta_{k,\alpha})t^\dagger_{-k,\alpha},$$
$$a^\dagger_{-k,\alpha} = \sinh(\theta_{k,\alpha})t_{k,\alpha} + \cosh(\theta_{k,\alpha})t^\dagger_{-k,\alpha}, \tag{8}$$

where k is the momentum and

$$\theta_{k,x} = \theta_{k,y} = \frac{2f_x(k)}{d_x(k)}; \qquad \theta_{k,z} = \frac{2f_z(k)}{d_z(k)}. \tag{9}$$

The functions $f_\alpha(k)$ and $d_\alpha(k)$ are defined in terms of the coupling constants by

$$f_x(k) = f_y(k) = \frac{t\bar{s}^2}{4}\gamma(k); \quad d_x(k) = d_y(k) = \mu + \frac{J_z}{4} + \frac{t\bar{s}^2}{2}\gamma(k),$$
$$f_z(k) = \frac{t\bar{s}^2}{4}\delta\gamma(k); \quad d_z(k) = \mu + \frac{2J_x - J_z}{4} + \frac{t\bar{s}^2}{2}\delta\gamma(k), \tag{10}$$

where $J_z = J\Delta$, $\gamma(k) = \sum_{i=1}^{D}\cos(k_i)$ and D is the dimension of rectangular Brillouin zone (BZ) associated with the D-dimensional rectangular lattice. The bosonic excitation energies in Eq. (7) are obtained as

$$\omega_\alpha(k) = \sqrt{d_\alpha^2(k) - 4f_\alpha^2(k)}, \qquad \alpha = x, y, z. \tag{11}$$

The ground state energy in D dimension is then given by

$$E_0 = N\left(\mu(\bar{s}^2 - 1) - (\frac{2J_x + J_z}{4})\bar{s}^2\right) + \frac{1}{2}\sum_k \sum_{\alpha=x,y,z}\left(\omega_\alpha(k) - d_\alpha(k)\right). \tag{12}$$

Minimization with respect to μ and $\bar{s}$ implies

$$\frac{\partial E_0}{\partial \mu} = 0, \qquad \frac{\partial E_0}{\partial \bar{s}} = 0. \tag{13}$$

Explicitly this leads to

$$\frac{1}{2N}\sum_{k\alpha}\frac{d_\alpha(k)}{\omega_\alpha(k)} = (\frac{5}{2} - \bar{s}^2)$$
$$\frac{t}{2N}\sum_{k\alpha}[\frac{d_\alpha(k) - 2f_\alpha(k)}{\omega_\alpha(k)}\gamma_\alpha(k)] = 2J_x[\frac{1}{2}(1 + \frac{J_z}{2J_x}) - \frac{\mu}{J_x}]. \tag{14}$$

Here we defined $\gamma_{x,y}(k) = \gamma(k)$ and $\gamma_z(k) = \delta\gamma(k)$. These equations will be solved selfconsistently for the average Kondo singlet amplitude $\bar{s}$ and the chemical potential μ. It is worthwile to write the m.f. Hamiltonian Eq.(7) in a different form as

$$H_{mf} = \tilde{E}_0 + \sum_k \sum_{\alpha=x,y,z}\omega_\alpha(k)(a^\dagger_{k,\alpha}a_{k,\alpha} + \frac{1}{2})$$
$$\tilde{E}_0 = -N\left(\frac{2J_x + J_z}{4}(\bar{s}^2 + \frac{1}{2}) + \mu(\frac{5}{2} - \bar{s}^2)\right) \tag{15}$$

Because $\bar{s} \leq 1$ the first part ($\tilde{E}_0$) is always negative and represents the m.f. singlet condensation energy. The second part is the (positive) energy of excited triplet bosons. The ground state has only a contribution from zero point motion. Both m.f. condensation energy and energy of zero point quantum fluctuations contribute to the total energy. Their balance determines the critical t_c for the quantum phase transition where the zero point fluctuation amplitude of bosons diverges, i.e., $\omega_\alpha(Q)$ becomes soft.

IV. NUMERICAL RESULTS: THE QUANTUM CRITICAL PHASE DIAGRAMS

We will now obtain the numerical solutions to the coupled equations (13). For this purpose we first consider the XY- case, i.e., $\delta = 0$ and arbitrary anisotropy Δ for the Kondo term in Eq. (1). We remind that in D=1 the XY-case is equivalent to the genuine Kondo lattice model with free itinerant electrons of a band-width W=4t. Later we will also investigate the case of nonzero δ.
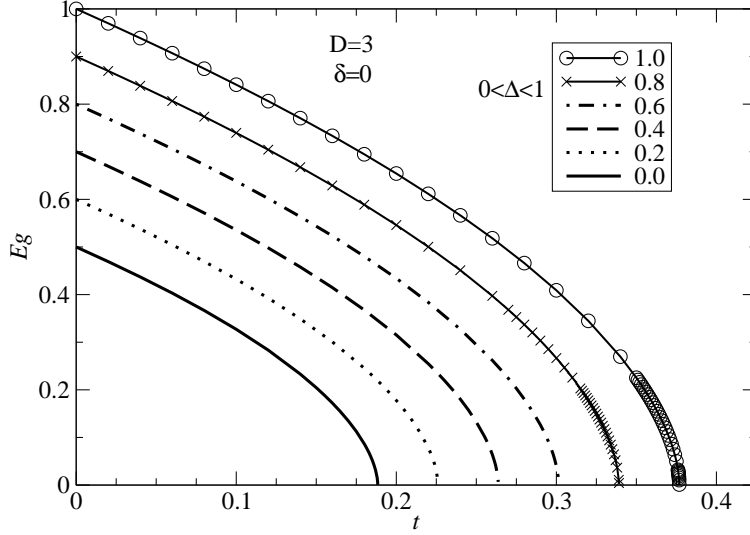
FIG. 4: The energy gap E_g versus hopping strength in the three dimensional lattice. The gap scales like $E_g \sim |t - t_c|^\nu$ with $\nu \simeq 0.55$.

A. XY-case: $\delta = 0$

In this case the z-polarised branch of excitations has a dispersionless value $\omega_z(k) = \omega_0$. However, the other two branches of excitations ($\omega_x = \omega_y$) show a dispersion which has a minimum at the antiferromagnetic reciprocal vector at the corner of the BZ, e.g., Q=(π,π) for D=2. The minimum value of excitations defines the energy gap

$$E_g = (\mu + \frac{J_z}{4})\sqrt{1 - D(\frac{t\bar{s}^2}{\mu + J_z/4})}. \tag{16}$$

In the present case the energy gap depends on the two parameters t and J_z. The gap E_g defines the energy scale for the Kondo singlet phase. When this energy scale approaches zero the other type of excitations become important and the model will encounter a phase transition from Kondo singlet to the antiferromagnetic phase. We will see that there exists a critical value for $t = t_c$ where this phase transition occurs in $D = 2, 3$ while no transition happens in $D = 1$. This is similar to the results in Ref. 7 for the special case $(\delta,\Delta)=(0,1)$ and to the previous results of MC simulations [8] for the 1D model. We have solved the mean field equations (13) numerically for general values of the coupling constants (t, J) and anisotropies (δ, Δ). The resulting value of μ and $\bar{s}$ are replaced in Eq.(16) to obtain the energy gap and track the location t_c where it vanishes.

In Fig.1 we have plotted the energy gap versus t (the hopping strength) for different anisotropies $0 \le \Delta = \frac{J_z}{J_x} \le 1$ in $D = 1$. The value of gap is reduced by decreasing the anisotropy from the isotropic ($\Delta = 1$) case to the XY-type ($\Delta = 0$) Kondo interaction. However, it is always nonzero and never vanishes. Thus, the effect of anisotropy does not change the universality behavior of the $D = 1$ case where the system is always in the Kondo singlet phase. We have also considered values with $\Delta > 1$ (easy axis- or Ising-type regime) and found a similar behavior as in Fig.1, provided we change the energy scale from J_x to J_z. It can be seen from the expression for the energy gap that there is a duality between the $0 \le \Delta \le 1$ and $\Delta > 1$ regions by interchanging $J_x \longleftrightarrow J_z$. For theoretical reasons we might also consider the negative values of anisotropy ($-1 \le \Delta \le 0$). Its behavior is similar to Fig.1 while the minimum of gap is reduced and vanishes at $t = 0$ for $\Delta = -1$. Actually, at $\Delta = -1$ the energy difference of the local singlet and the two triplet states becomes zero which leads to the vanishing of the energy gap. However, in this limit the above mean field approach is not reliable where the triplet contribution can not be neglected in the ground state. For negative values of Δ the average value of the triplets is comparable with the singlets and should be taken into account on the same footing.
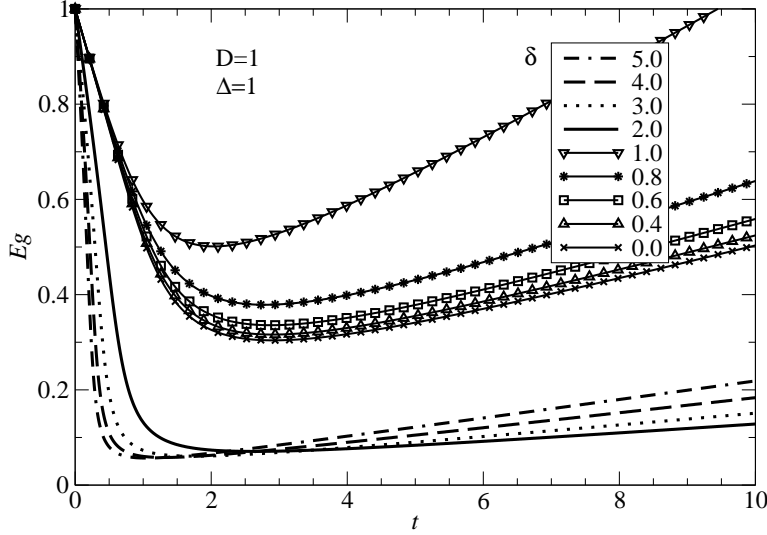
FIG. 5: The energy gap versus t for different values of δ in the one dimensional lattice. The gap is always nonzero for $\delta \geq 0$.

Let us now present the results for the square lattice ($D = 2$) shown in Fig.2. We have plotted the energy gap versus t for different values of $0 \leq \Delta \leq 1$. For all values of Δ the gap vanishes at the critical point t_c, where the transition from Kondo singlet to the antiferromagnetic phase occurs. The dependence of the critical point on the anisotropy is linear and is fitted well by $t_c \simeq 0.35J(\Delta + 1)$ which is also valid for negative values of $-1 \leq \Delta \leq 0$ but has not been shown here. We will derive an equation for the critical temperature of $D = 2, 3$ in terms of the coupling parameters in Sec. V. The linear dependence of t_c on Δ shows that the anisotropy term is important to stabilize the Kondo singlets. Thus, for higher Δ, higher value of the hopping term is required to destroy the Kondo singlet and induce the antiferromagnetic order. However, the qualitative behavior of the energy gap versus t is the same for all Δ. Our fine tuned data plotted in the inset of Fig.2 show that the gap vanishes close to t_c with a critical exponent ν according to

$$E_g \sim |t - t_c|^{\nu}, \tag{17}$$

where $\nu \simeq 1$ for $D = 2$. The exponent is the same for all anisotropies and this is in agreement with the observation that the local interaction terms will not change the universal behavior. The log-log plot of E_g versus $|t - t_c|$ for all Δ fall on each other which justifies the scaling behaviour close to critical point. The extension of our calculation to $\Delta > 1$ (Ising regime) shows qualitatively similar results. We have also plotted the value of $\bar{s} = <s>$ versus the hopping term in Fig. 3 for two different values of anisotropy, $\Delta = 0, 1$ in the case of two dimensional square lattice. These data justify our assumption that the expectation value of singlets in the ground state is close to one up to the critical t_c value. It supports our claim to neglect the occupation of triplets in the ground state in the mean field approach.

Our results for $D = 3$ are shown in Fig. 4. The gap versus t shows similar behavior qualitatively for all values of Δ. There exists always a critical point (t_c) which shows the transition from Kondo singlet to the antiferromagnetic phase. The critical point depends on the anisotropy linearly, $t_c \simeq 0.188J(\Delta + 1)$. The exact expression for the critical point is given by an equation in Sec.V. However, the dependence is weaker than in the case of $D = 2$. The reason is related to the increase of the number of nearest neighbor sites which allows hopping more easily. Thus, the hopping term is more effective here. The analysis of log-log plot of Fig. 4 close to the critical point gives the gap exponent to be $\nu \simeq 0.55$ for the three dimensional cubic lattice.
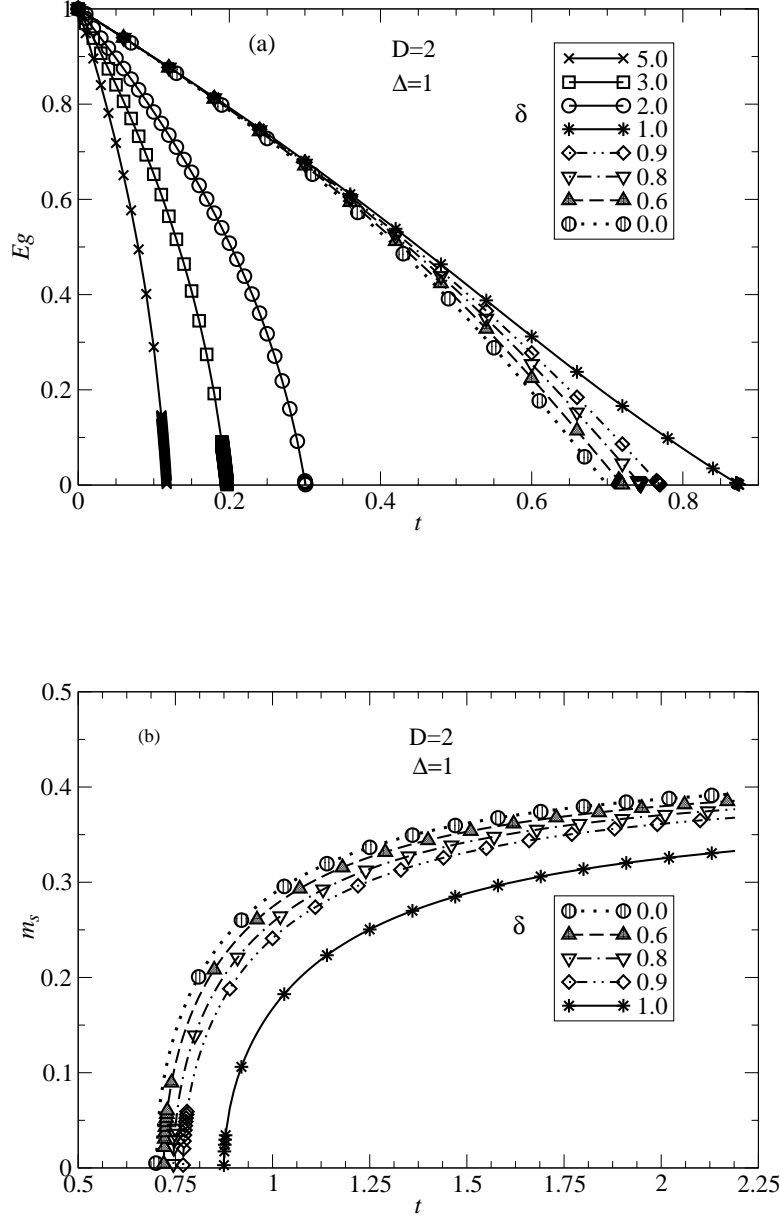
FIG. 6: Two dimensional lattice: (a) The behavior of gap for two different regimes of δ versus t in two dimensional lattice for $\Delta = 1$. The scaling of gap close to the critical hopping (t_c) is obviously different for $0 \leq \delta \leq 1$ and $\delta > 1$, ($\delta = 2, 3, 5$). (b) Staggered magnetization (m_s) versus t in the antiferromagnetic phase, just above the quantum critical point at t_c. The local anisotropy is $\Delta = 1$ and the itinerant one varies within $0 \leq \delta \leq 1$.

B. general ansisotropic case $\delta \neq 0$

Our results in the previous case, $\delta = 0$, show that the anisotropy in the local interaction (Δ) does not change the qualitative behavior of the necklace model on the cubic lattices with D=1-3. In order to study the effect of a nonzero anisotropy $\delta \neq 0$ in the 'itinerant' part ($\sim t$) in Eq. (1) it is therefore sufficient to consider only the isotropic case of the local Kondo interactions, i.e., $J_x = J_z = J$, ($\Delta = 1$).
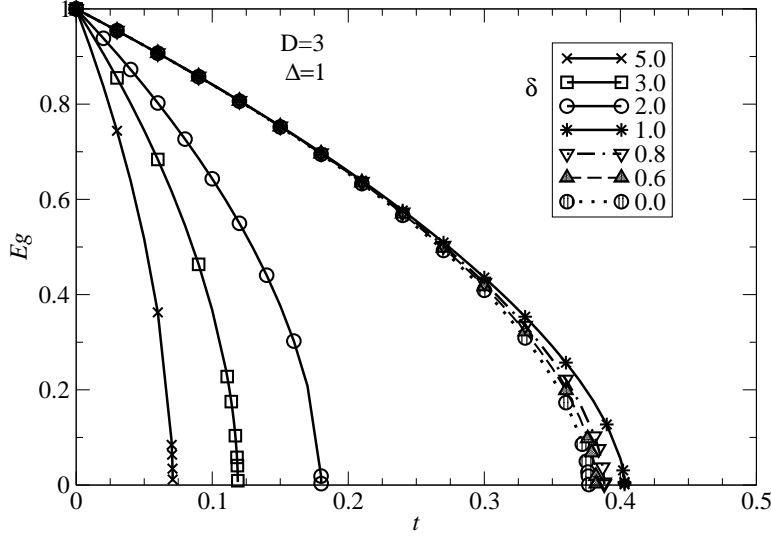
FIG. 7: The effect of δ on the behavior of gap versus t for the three dimensional cubic lattice. The gap vanishes at the critical point with different scaling behavior for $0 \leq \delta \leq 1$ and $\delta > 1, (\delta = 2, 3, 5)$.

When δ is nonzero, we find three excitation modes in Eq.(11) which now all show dispersion. The minimum of excitations which introduces the energy gap appears again at the antiferromagnetic reciprocal wave vector Q. In contrast to the previous case, the excitation in z-direction (ω_z) is important and defines the gap for the easy-axis type anisotropy $\delta > 1$. The minimum excitation energies for the modes at Q are given by

$$E_g^x = E_g^y = (\mu + \frac{J}{4})\sqrt{1 - D(\frac{t\bar{s}^2}{\mu + J/4})},$$

$$E_g^z = (\mu + \frac{J}{4})\sqrt{1 - \delta D(\frac{t\bar{s}^2}{\mu + J/4})}. \tag{18}$$

For $0 \leq \delta < 1$, we have $E_g^x < E_g^z$. However, at $\delta = 1$ the energy gap of all excitations coincide. If we consider $\delta > 1$ the situation is reversed and $E_g^z < E_g^x$. This is important because the vanishing of gap and the appearance of soft modes define the transition from Kondo singlet to the antiferromagnetic phase.

In the case of one dimensional space ($D = 1$) the energy gap is always nonzero for $0 \leq \delta \leq 1$. The dependence of the gap on the anisotropy of the 'itinerant' term (δ) in Eq.(1) is smooth as shown in in Fig.5. However, there is an abrupt change in the value of gap at $\delta = 1$ which is related to the contribution of the third soft mode (ω_z) to the lowest energy part of the model. The situation is almost the same for $\delta > 1$ where the gap never vanishes and therefore no phase transition appears for increasing t.

The effect of δ anisotropy in the two dimensional lattice is plotted in Fig.6(a). As discussed earlier the gap E_g is defined by the E_g^x and E_g^y for $0 \leq \delta \leq 1$ and E_g^z for $\delta > 1, (\delta = 2, 3, 5)$. For $\delta < 1$ the effect of anisotropy is weak and it changes the critical point (t_c) slightly. The dependence of the critical point (t_c) is not a simple function as will be given in the next section. The qualitative behavior is the same for all $\delta < 1$ and the gap exponent is approximately $\nu \simeq 1$. We observe a jump in the critical point which appears at $\delta = 1$. Because at this point another soft mode (ω_z) is added to the excitations at the critical point which needs a larger hopping strength t to overcome them. If we describe the gap close to the critical point by $E_g = A(\delta)|t - t_c|^\nu$ the coefficient $A(\delta = 1)$ is almost half the value for the other cases ($A(\delta \neq 1)$). When $\delta > 1$, t_c is reduced and the Kondo singlet phase is limited to a smaller region. In this case the interaction between the itinerant electron ($t\delta$) dominates the Kondo term (J) for smaller values of t. The change of universality in approaching the critical point is also obvious from Fig.6(a).

Increasing t beyond t_c leads to antiferromagnetic order as discussed in Sect. V. For comparison we have also plotted the AF order parameter (staggered magnetization) versus t in Fig.6(b). The staggered magnetization is zero in the singlet phase until $t = t_c$. For high values of t ($t \gg J$), the antiferromagnetic order parameter is close to saturation. The reduction of t increases the effect of the local exchange interaction which favors the singlet phase. At the critical point ($t = t_c$) the staggered magnetization is destroyed by the AF fluctuations connected with the soft modes. This happens exactly at the point where the Kondo singlet energy gap mentioned in previous paragraph vanishes.

We also show the effect of nonzero δ on the three dimensional cubic lattice in Fig.7. As discussed earlier, the minimum of excitations in x- or y-direction gives the scale of energy (E_g^x, E_g^y) for $0 \le \delta \le 1$ and E_g^z for $\delta > 1$. The effect of δ on the behavior of energy gap versus t is weaker than the case of $D = 2$. The gap vanishes at the critical point which has a slight dependence on δ. There is a jump on the critical point at $\delta = 1$ which is the result of three soft modes at this point while for $0 \le \delta \le 1$ there are two soft modes and for $\delta > 1$ only one soft mode. Although δ is a global term in the interaction there is no change in the scaling behavior of the gap close to the critical point. The gap exponent for $0 < \delta \le 1$ is the same as for zero δ, namely $\nu \simeq 0.55$. However, we have observed different behavior for $\delta > 1$ where the gap vanishes close to critical point more rapidly. But we were not able to find a scaling exponent in this regime because here t_c varies too strongly with δ. In the other cases we have determined the scaling exponents numerically from the selfconsistent solutions and found them to lie close to $\nu = \frac{1}{2}$ for 2D and $\nu = 1$ for 3D. The deviations are mostly due to the numerical inaccuracy of t_c determination. This is the expected result for the present mean field approach. In the special case $(\delta, \Delta) = (0,1)$ we have expanded the selfconsistent equations Eq.(14) around $E_g = 0$ which indeed leads to the analytical mean field scaling behaviour for E_g.

V. ANTIFERROMAGNETIC PHASE

The mean field approach can be simply extended to the antiferromagnetic phase for $D = 2, 3$. For large enough t/J the long range antiferromagnetic order sets up which means the condensation of a component of local spin triplets. We assume the condensation in the x-component of the spin triplet ($t_{k,x}$) at the antiferromagnetic wave vector ($Q = (\pi, \pi)$ for D=2),

$$t_{k,x} = \sqrt{N}\bar{t}\delta_{k,Q} + \eta_{k,x}. \tag{19}$$

In Eq.(19) $\bar{t}$ is the mean value of the x-component of the spin triplet in the ground state and $\eta_{k,x}$ is its quantum fluctuations. We replace $t_{k,x}$ into the Fourier trasformed of Eq.(6) to derive the mean field Hamiltonian assuming $\langle s_k \rangle = \bar{s}$ and $\langle t_{k,x} \rangle = \bar{t}$. The mean field Hamiltonian will be in the following form,

$$H^{AF} = E_0^{AF} + \sum_k \omega_z(k) t_{k,z}^\dagger t_{k,z} + \sum_k \omega_x(k)(\tilde{\eta}_k^\dagger \tilde{\eta}_k + \tilde{t}_{k,y}^\dagger \tilde{t}_{k,y}), \tag{20}$$

where $\tilde{O}$ represent the new operators after Bogoliubov transformation. The ground state energy (E_0^{AF}) is defined below,

$$E_0^{AF} = E_0 + N\bar{t}^2(\mu + \frac{J_z}{4} - Dt\bar{s}^2), \tag{21}$$

where E_0 has been defined in Eq.(12). The ground state energy E_0^{AF} is minimized with respect to μ, $\bar{s}$ and $\bar{t}$ which leads to the following equations,

$$\begin{aligned}
\mu &= Dt\bar{s}^2 - \frac{J_z}{4}, \\
\bar{s}^2 &= \frac{5}{4} + \frac{J_x + J_z}{4Dt} - \frac{1}{2N}\sum_k \sqrt{1 + \frac{\gamma(k)}{D}} - \frac{1}{4N}\sum_k \frac{X_+^k}{\omega_z(k)} \\
\bar{t}^2 &= \frac{5}{4} - \frac{J_x + J_z}{4Dt} - \frac{1}{2N}\sum_k \frac{1}{\sqrt{1 + \frac{\gamma(k)}{D}}} - \frac{1}{4N}\sum_k \frac{X_-^k}{\omega_z(k)}.
\end{aligned} \tag{22}$$

Furthermore,

$$\begin{aligned}
X_+^k &= \frac{1}{2}(J_x - J_z)(1 + \delta\frac{\gamma(k)}{2D}) + Dt\bar{s}^2(1 + \delta\frac{\gamma(k)}{D}), \\
X_-^k &= \frac{1}{2}(J_x - J_z)(1 - \delta\frac{\gamma(k)}{2D}) + Dt\bar{s}^2.
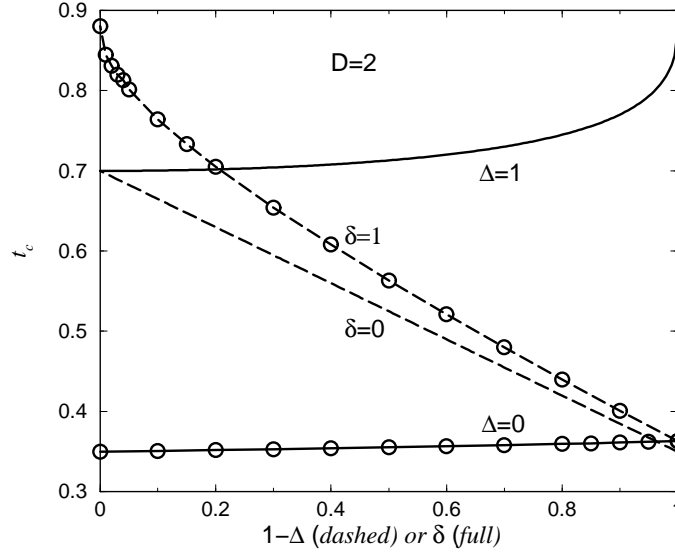\end{aligned} \tag{23}$$

FIG. 8: Dependence of the quantum critical point t_c (in units of J_x) for $D = 2$ on itinerant (δ, full line) and local (1-Δ, dashed line) anisotropy parameters. The lines without symbols are from the closed analytical form in Eq.(25), the curves with symbols are obtained from numerical solution Eq.(22) or Eq.(14).

Generally the equation for $\bar{s}$ should be solved selfconsistently and then μ and $\bar{t}$ can be found directly from the above equations. However, for $\Delta = 1$, the above equation (Eq.(22)) for $\bar{s}$ is simplified to a direct integral expression. If in addition $\delta = 0$ the result in Ref.7 is recovered. For the bipartite lattice which we have assumed the antiferromagnetic order parameter is defined on A- or B-sublattices as,

$$\langle S_x \rangle_A = -\langle S_x \rangle_B = \bar{s}\bar{t}, \tag{24}$$

Here $m_s = \bar{s}\bar{t}$ is the staggered moment. It is plotted for $D = 2$ and different δ values in Fig. 6(b). The appearance of long range antiferromagnetic order (nonzero m_s) defines the quantum critical point $t = t_c$. This is identical to the value where the Kondo singlet gap vanishes as seen in the conjugate plot in Fig. 6(a). The formulation presented in this section allows us to obtain an explicit expression for the critical point (t_c) for the special cases $(\delta, \Delta) = (0, \Delta)$ and $(\delta, \Delta) = (\delta, 1)$ which is given by

$$\frac{1}{t_c} = \Big(\frac{2D}{1+\Delta}\Big)\Big(\frac{5}{2} - \frac{1}{2N}\sum_{k,\alpha} \frac{1}{\sqrt{1 + \frac{\gamma_\alpha(k)}{D}}}\Big). \tag{25}$$

Here we used again $\gamma_{x,y}(k) = \gamma(k)$ and $\gamma_z(k) = \delta\gamma(k)$. For the other cases one has to obtain t_c numerically by the selfconsistent solution of Eq.(22) or equivalently by Eq.(14). For D=2 we have plotted the value of t_c versus $1 - \Delta$ (at fixed $\delta = 0$) or versus δ (at fixed $\Delta = 1$) in Fig. 8. The bare lines correspond to the analytical solution of Eq.(25) while the lines with symbols correspond to the numerical solution for t_c. One notices that on approaching $(\delta, \Delta) \to (1,1)$ where $t_c=0.88$ (the two uppermost points in Fig. 8) the slope of $t_c(\Delta)$ or $t_c(\delta)$ diverges. This signifies the change of universality class from U(1) to SU(2) at the point $(\delta, \Delta)=(1,1)$ which leads to the apperance of a third soft mode at t_c.

VI. SUMMARY AND DISCUSSIONS

We have studied the quantum critical properties of the fully anisotropic Kondo-necklace model in dimension D=1-3. We used the bond-operator representation of spin variables with constraints implemented in the mean field approximation. For general anisotropy ratios (δ, Δ) we have calculated the critical values $(t/J)_c$ and the scaling exponenets of the Kondo singlet gap close to the quantum critical point which correspond to the mean field exponents.

We find that in general the anisotropy Δ of the local Kondo term influences the qualitative behavior of the singlet gap only little, although the value of the critical ratio $(t/J)_c$ depends strongly on Δ. If Δ decreases the Kondo singlet

is destabilized and the critical value $(t/J)_c$ decreases. On the other hand the anisotropy of the inter-site term which mimics the itinerant electrons has a weak effect on the position of the critical point (Fig. 8) and leaves the universal behavior similar as in the conventional XY-type ($\delta = 0$) Kondo necklace model. On approaching the SU(2) Heisenberg case (δ, Δ)=(1,1) t_c exhibits a singular behaviour as function of anisotropies. This is most pronounced in D=2 where also the scaling coefficient (not the exponent) of the gap close to the QCP changes considerably as compared to the $\delta = 0$ case. Furthermore the value of the critical $(t/J)_c$ with properly defined scale J exhibits a jump at δ=1. This peculiar effect is due to a mode crossing of the x,y and z branches of excitations at the AF wave vector as function of δ.

We have also derived and solved the selfconsistency equations on the magnetic side for general (δ, Δ). This allows us to give an explicit expression for the quantum critical point value t_c as function of anisotropy parameters (δ, Δ) for the cases δ=0 or Δ=1 for dimension D=2,3. To discuss the scaling exponents beyond mean field approximation the renormalisation of triplet excitation energies close to the QCP caused by fluctuations in the bosonic variables has to be included.

VII.   ACKNOWLEDGMENT

VIII.   APPENDIX

The explicit form of H_2 and H_3 introduced in Sect. III in terms of bond operators are as follows:

$$
H_2 = \frac{-t}{4} \sum_{\langle n,m \rangle} \Big((t_{n,y}^{\dagger} t_{n,z} - h.c.)(t_{m,y}^{\dagger} t_{m,z} - h.c.) + (t_{n,x}^{\dagger} t_{n,z} - h.c.)(t_{m,x}^{\dagger} t_{m,z} - h.c.)
$$
$$
+ \ \delta(t_{n,x}^{\dagger} t_{n,y} - h.c.)(t_{m,x}^{\dagger} t_{m,y} - h.c.) \Big). \tag{26}
$$

The terms appearing in H_2 describe the interaction between triplets. Since the triplet occupation is very small in the ground state, the effect of H_2 on the mean field result is negligible.

The remaining part of H_t is expressed by H_3 which gives zero contribution to the ground state energy in the mean field approximation.

$$
H_3 = \frac{it}{4} \sum_{\langle n,m \rangle} \Big([(s_n^{\dagger} t_{n,x} + t_{n,x}^{\dagger} s_n)(t_{m,y}^{\dagger} t_{m,z} - t_{m,z}^{\dagger} t_{m,y}) + (s_n^{\dagger} t_{n,y} + t_{n,y}^{\dagger} s_n)(t_{m,z}^{\dagger} t_{m,x} - t_{m,x}^{\dagger} t_{m,z})
$$
$$
+ \ \delta(s_n^{\dagger} t_{n,z} + t_{n,z}^{\dagger} s_n)(t_{m,x}^{\dagger} t_{m,y} - t_{m,y}^{\dagger} t_{m,x})] + h.c. \Big). \tag{27}
$$

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